Symplectic Integration for the Transport Properties of Simple Fluids

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In this study we have investigated the transport properties of fluids using symplectic integration (SI) algorithms for the equations of motion. In particular, an extensive series of equilibrium molecular dynamic simulations have been performed to investigate the accuracy, stability and efficiency of second order explicit symplectic integrators: position Verlet, velocity Verlet, and the McLauchlan-Atela algorithms. Comparisons have been made to non-symplectic integrators that include the fourth order Runge-Kutta and fourth order Gear predictor-corrector methods. These comparisons were performed based on several transport properties of Lennard-Jones fluids: self-diffusion, shear viscosity and thermal conductivity. Because transport properties involve long time simulations to obtain accurate evaluations of their numerical values, they provide an excellent basis to study the accuracy and stability of the SI methods. To our knowledge, previous studies on the SIs have only looked at the thermodynamic energy using a simple model fluid. Our work presents realistic but perhaps the simplest simulations possible to test the effect of the integrators on the three main transport properties. Our results suggest that if an algorithm fails to conserve energy adequately, it will also show significant uncertainties in transport property calculations.